

National Institute of Standards & Technology

Certificate of Analysis

Standard Reference Material® 2519a

High Resolution Wavelength Calibration Reference for 1530 nm - 1565 nm Hydrogen Cyanide $\mathrm{H}^{13}\mathrm{C}^{14}\mathrm{N}$

Serial No.:

This Standard Reference Material (SRM) is intended for wavelength calibration in the spectral region from 1530 nm to 1565 nm; the center wavelengths of 54 lines of the $2\nu_3$ rotational-vibrational band of hydrogen cyanide $H^{13}C^{14}N$ are certified. This SRM can be used for calibrating a variety of wavelength-measuring instruments such as optical spectrum analyzers, tunable lasers, and wavelength meters. SRM 2519a is a single-mode optical-fiber-coupled absorption cell containing hydrogen cyanide $H^{13}C^{14}N$ gas at a pressure of 3.3 kPa (25 Torr). The absorption path length is 15 cm and the absorption lines are about 15 pm wide. The cell is packaged in a small instrument box (approximately 32 cm long x 12.5 cm wide x 9 cm high) with two FC/APC fiber connectors for the input and output of a user-supplied light source. The main difference between SRM 2519a and its predecessor, SRM 2519, is the use of lower pressure in the hydrogen cyanide cell to produce narrower lines. Thus, SRM 2519a extends the use to higher resolution and higher accuracy applications.

Certified Wavelength Values: The line centers, pressure shift, and pressure broadening for 25 lines in the $\rm H^{13}C^{14}N\ 2v_3$ rotational-vibrational combination band have been accurately measured at NIST, and the molecular constants of the band have been determined [1]. The certified line center for each of the 25 lines measured at NIST was determined by adding the line's pressure shift (due to collisions between HCN molecules at the 3.3 kPa pressure within the SRM cell) to the measured zero-pressure line center. The zero-pressure line centers of other lines in the band were calculated from the molecular constants of the band, and the appropriate pressure shift was derived using interpolation and extrapolation [2]. Details of the measurement procedure, data analysis, and uncertainty analysis can be found in references 1 and 2. A spectrum of the absorption band is shown in Figure 1, and certified wavelength values are given in Table 1. Figures 2–4 show scans near lines P10, P11, and P16. The center wavelengths of the lines listed in Table 1 are certified with uncertainties ranging from 0.04 pm to 0.24 pm. These uncertainties are the expanded uncertainties using a coverage factor k = 2 (i.e., our quoted uncertainty is $\pm 2\sigma$).

Expiration of Certification: The certification of this SRM is indefinite within the measurement uncertainties specified, provided the SRM is handled, stored, and used in accordance with the instructions given in this certificate (see "Storage and Handling").

The coordination of the development of the SRM and supporting measurements were performed by W.C. Swann and S.L. Gilbert of the NIST Optoelectronics Division.

Statistical consultation was provided by C.M. Wang of the NIST Statistical Engineering Division.

The support aspects involved in the preparation, certification, and issuance of this SRM were coordinated through the NIST Standard Reference Materials Program by C.S. Davis of the NIST Measurement Services Division.

Kent B. Rochford, Chief Optoelectronics Division

Robert L. Watters, Jr., Chief Measurement Services Division

Gaithersburg, MD 20899 Certificate Issue Date: 11 April 2005

Table 1. Certified Wavelengths for SRM 2519a

R Branch	Wavelength (nm)	P Branch	Wavelength (nm)
26	1527.63342(12)	1	1543.11423(5)
25	1528.05474(15)	2	1543.80967(18)
24	1528.48574(9)	3	1544.51503(8)
23	1528.92643(6)	4	1545.23033(7)
22	1529.37681(7)	5	1545.95549(7)
21	1529.83688(6)	6	1546.69055(8)
20	1530.30666(8)	7	1547.43558(24)
19	1530.78615(8)	8	1548.19057(7)
18	1531.27537(7)	9	1548.95555(4)
· 17	1531.77430(8)	10	1549.73051(4)
16	1532.28298(8)	11	1550.51546(5)
15	1532.80139(7)	12	1551.31045(9)
14	1533.32954(8)	13	1552.11546(10)
. 13	1533.86745(7)	14	1552.93051(9)
12	1534.41514(6)	15	1553.75562(12)
11	1534.97258(6)	16	1554.59079(10)
10	1535.53981(5)	. 17	1555.43605(11)
9	1536.11683(4)	18	1556.29141(15)
8	1536.70364(5)	19	1557.15686(15)
7	1537.30029(6)	20	1558.03240(15)
6	1537.90675(13)	21	1558.91808(14)
5	1538.52305(7)	22	1559.81389(14)
4 .	1539.14921(12)	23	1560.71983(10)
3	1539.78523(9)	. 24	1561.63593(9)
2	1540.43120(10)	25	1562.56218(13)
1	1541.08703(10)	26	1563.49859(16)
0	1541.75280(6)	27	1564.44519(21)
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Certified vacuum wavelengths of line centers in the $\mathrm{H}^{13}\mathrm{C}^{14}\mathrm{N}$ $2\nu_3$ rotational-vibrational band at the SRM pressure of 3.3 kPa (25 Torr). Line centers are certified with the uncertainty indicated in parenthesis for the last digits. The uncertainties quoted are the expanded uncertainty using a coverage factor k=2 (i.e., our quoted uncertainty is $\pm 2\sigma$).

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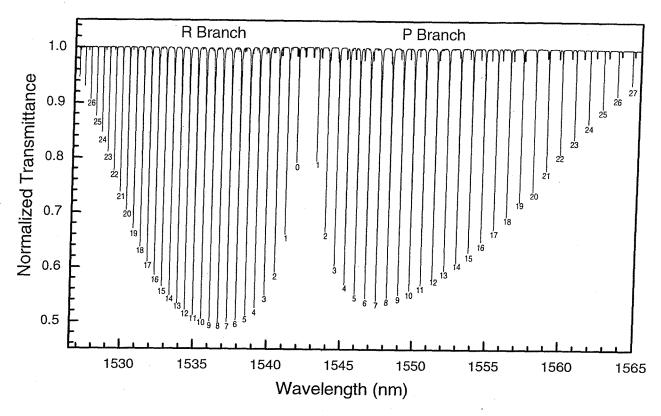


Figure 1. Normalized spectrum of the hydrogen cyanide $H^{13}C^{14}N$ $2v_3$ band obtained by scanning a tunable diode laser (~1 MHz linewidth) and measuring the laser power transmitted through a SRM unit. The SRM contains a 15 cm long absorption cell filled with $H^{13}C^{14}N$ to a pressure of 3.3 kPa (25 Torr). A file containing these data can be downloaded from NIST at http://ts.nist.gov/srmcertificate/?srm=2519.

Storage and Handling: The protective caps provided for the FC/APC fiber connectors should be replaced when the SRM is not in use. This SRM is intended to be used in a laboratory environment near ambient room temperature (22 °C \pm 5 °C). The user should avoid exposing the unit to large temperature variations, temperature cycling, or mechanical shock, as these may cause the optical alignment to degrade. Such optical misalignment affects the throughput of the SRM but will not shift the centers of the absorption lines.

Maintenance of SRM Certification: The gas is contained in a glass cell with all-glass seals at the windows and the fill port. In the unlikely event of cell leakage, the linewidths and the small pressure shift of the line centers will change. Contact NIST if the linewidths or depths differ significantly from those shown in Figures 1–3, when measured with comparable resolution (see specific criteria in the section Suggested Procedure for High-Accuracy Requirements). If substantive changes occur that affect the certification, NIST will notify the purchaser. Registration (see attached sheet) will facilitate notification.

Certification Measurement Conditions and Procedure: The long term stability of hydrogen cyanide and the use of fundamental molecular absorption lines render the SRM insensitive to changes in environmental conditions. The purpose of the certification procedure is to verify that the unit contains the correct pressure of H¹³C¹⁴N gas, has no significant contaminants, and shows no evidence of cell leakage. Measurements of the spectral band, similar to that shown in Figure 1, are made using a broadband source and an optical spectrum analyzer. Higher resolution measurements are made using a tunable diode laser (~1 MHz linewidth) and a calibrated wavelength meter; spectra similar to that shown in Figure 2 are taken of each SRM unit and one or more lines are accurately fit to verify the line's center and width using the procedure described in reference [1]. To test for cell leakage, the higher resolution measurements are repeated after a minimum waiting period of one month.

INSTRUCTIONS FOR USE

General Considerations: The SRM can be used to calibrate a laser or wavelength-measuring instrument in the 1530 nm to 1565 nm region. The values in Table 1 are vacuum wavelengths; if the user requires the wavelength in air, the appropriate correction for the index of refraction of air must be applied [3]. Depending on what type of instrument is being calibrated, a user-supplied broadband source or a tunable narrowband source may be used. Typical optical connections are shown in Figure 5. The unit is bi-directional (has no preferred input/output port); connections to the unit should be made using single-mode optical fibers terminated with clean FC/APC connectors.

Use With a Broadband Source: A broadband source in the 1530 nm – 1565 nm region (such as a light emitting diode, white light, or amplified spontaneous emission source) is useful when calibrating an instrument such as a diffraction grating based optical spectrum analyzer. A schematic for this type of calibration is shown in Figure 5(a). Light from the broadband source is coupled into the SRM, and the output (transmission through the SRM) is connected to the instrument that is being calibrated. The absorption lines of hydrogen cyanide appear as dips in the spectrum of the light source.

Use With a Tunable Source: The SRM can be used to calibrate the wavelength scale of a tunable source in this region (such as a diode laser, a fiber laser, or a source filtered by a tunable filter). A schematic for this type of calibration is shown in Figure 5(b). The laser is tuned over one or more of the hydrogen cyanide absorption lines. The transmission through the SRM is monitored by a detector; the transmitted power passes through a minimum at the center of an absorption line. Alternatively, a tunable laser source and the SRM can be used to check the calibration of a wavelength meter by measuring the wavelength of the laser (using the wavelength meter) as the laser is tuned through an absorption line.

Suggested Procedure for Low-Accuracy Requirements – Calibration Uncertainty > 30 pm: If calibrating an instrument using a broadband source, use an instrument resolution of ≤ 0.1 nm. If using a tunable source, use a data point density of at least one point every 0.005 nm (5 pm). After identifying a particular absorption line by comparing to the spectrum in Figure 1, find the center or minimum point of the line. Calibrate the instrument to the center wavelength of this line (from Table 1) using the calibration procedure specified by the instrument manufacturer. The instrument's linearity can be checked by repeating the procedure for a different absorption line and comparing it to the value listed in Table 1.

Suggested Procedure for Moderate-Accuracy Requirements – Calibration Uncertainty in the Approximate Range of 3 pm to 30 pm: If the source power varies significantly with wavelength, divide the SRM transmission spectrum by the source spectrum to obtain a normalized trace. After identifying a particular absorption line by comparing to the spectrum in Figure 1, make a high resolution scan of the line. If calibrating an instrument using a broadband source, use an instrument resolution of ≤ 0.05 nm. If using a tunable source, use a data point density of at least one point every 0.002 nm (2 pm). Find the wavelength readings on both sides of the line where the absorption is 50 % of the maximum; the line center is half way between these two wavelength readings. For higher accuracy results, repeat this procedure five times and take the average of the measurements. Calibrate the instrument to the center wavelength of this line (from Table 1) using the calibration procedure specified by the instrument manufacturer. The instrument's linearity can be checked by repeating the procedure for a different absorption line and comparing it to the value listed in Table 1.

NOTE: Highly reproducible *relative* wavelength measurements can be made using the procedure described for moderate-accuracy requirements. However, the procedure described in the following section is recommended to achieve high-accuracy *absolute* wavelength calibration.

Suggested Procedure for High-Accuracy Requirements – Calibration Uncertainty < 3 pm: Connect a narrowband tunable light source (source bandwidth ≤ 1 pm) to one of the fiber connectors on the SRM unit. After identifying a particular absorption line by comparing to the spectrum in Figure 1, make a high resolution scan of the line. To minimize polarization-dependent transmittance changes, avoid movement of the connecting fiber patchcords during the measurement. Use a data point density of at least one point every 1 pm and divide the SRM transmission spectrum by the source spectrum to obtain a normalized trace. Using a fitting technique such as the least squares technique, fit the absorption data to a Lorentzian or Voigt lineshape. Details of a line fitting procedure and potential errors sources can be found in reference 1, which is also included as an appendix in reference 2. Calibrate the instrument to the center wavelength of this line (from Table 1) using the calibration procedure specified by the instrument manufacturer. The instrument's linearity can be checked by repeating the procedure for a different absorption line and comparing it to the value listed in Table 1. Contact NIST if the width of line P16 differs by more than 25 % from the width shown in Figure 2, when measured using comparable resolution. A large change in linewidth could indicate cell leakage.

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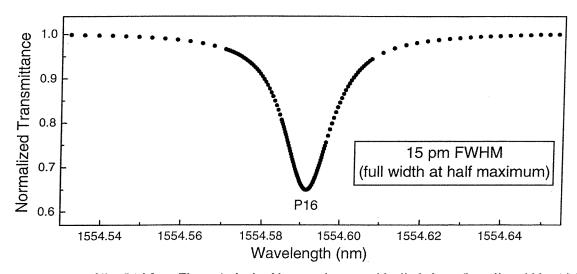


Figure 2. Spectrum of line P16 from Figure 1 obtained by scanning a tunable diode laser (laser linewidth ~1 MHz).

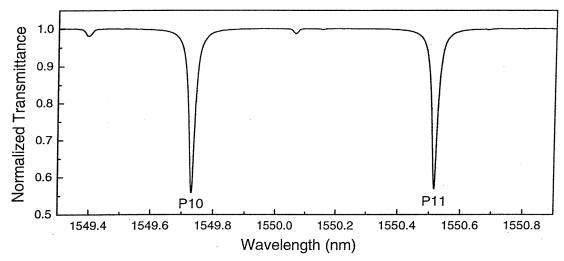


Figure 3. Spectrum of lines P10 and P11 from Figure 1 obtained by scanning a tunable diode laser.

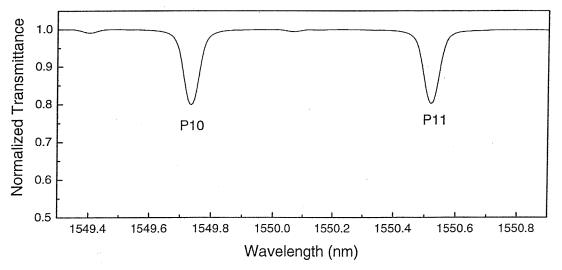


Figure 4. Spectrum of lines P10 and P11 obtained using a broadband source and an optical spectrum analyzer set to 0.05 nm resolution.

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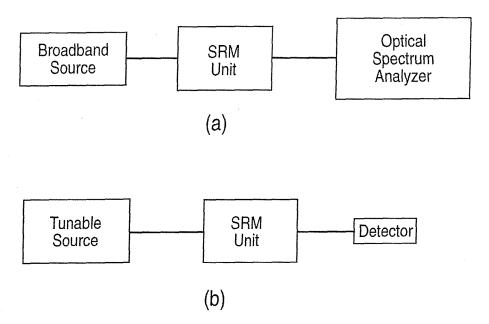


Figure 5. (a) Schematic of technique when using the SRM and a broadband source to calibrate an optical spectrum analyzer. (b) Schematic of technique when using the SRM to calibrate a tunable source. A wavelength meter can be calibrated by using a tunable laser in the configuration shown in (b) and measuring its wavelength using the wavelength meter.

REFERENCES

- [1] Swann, W.C.; Gilbert, S.L.; Line Centers, Pressure Shift, and Pressure Broadening of 1530–1560 nm Hydrogen Cyanide Wavelength Calibration Lines; J. Opt. Soc. Am. B. (2005) in press. Note: This paper is included as an appendix in reference [2] (below).
- [2] Gilbert, S.L.; Swann, W.C.; Hydrogen Cyanide H¹³C¹⁴N Absorption Reference for 1530 nm to 1565 nm Wavelength Calibration SRM 2519a; NIST Special Publication 260-137 2005 ed, in press.
- [3] Edlen, B.; The Refractive Index of Air; Metrologia, Vol. 2, p. 12 (1966); CRC Handbook of Chemistry and Physics 77th ed., pp. 10–266, (1996); Stone, J.A.; Zimmerman, J.H.; Index of Refraction of Air; http://patapsco.nist.gov/mel/div821/Wavelength/Documentation.asp#IndexofRefractionofAir.

Users of this SRM should ensure that the certificate in their possession is current. This can be accomplished by contacting the SRM Program at: telephone (301) 975-6776; fax (301) 926-4751; e-mail srminfo@nist.gov; or via the Internet at http://www.nist.gov/srm.